AMENDMENT

Please amend the above-captioned application as follows:

In the Claims:

Please amend the claims as follows:

45. (Twice amended) A computer program product comprising a computer useable medium having computer program logic recorded thereon for creating a functional site descriptor for use in predicting a biological function of a protein, said computer program logic comprising computer program code logic configured to perform the operations of:

(a) determining a set of geometric constraints for a functional site associated with a biological function of a protein, wherein a set of geometric constraints comprises one or more geometric constraints between at least three different atoms, wherein each atom is in a different amino acid residue of the protein and the different atoms comprise:

(i) an atom of a first amino acid residue of the functional site comprising the amino acid residue of part (a), wherein the atom is selected from the group consisting of a backbone amide nitrogen, an alpha-carbon, a backbone carbonyl carbon, a backbone carbonyl oxygen, a backbone pseudoatom, and a beta-carbon;

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(ii) an atom of a second amino acid residue of the functional site, wherein the atom is selected from the group consisting of a backbone amide nitrogen, an alpha-carbon, a backbone carbonyl carbon, a backbone carbonyl oxygen, a backbone pseudoatom, and a beta-carbon; and

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(iii) an atom of a third amino acid residue of the protein, wherein the atom is selected from the group consisting of a backbone atom, a side chain atom, and a pseudoatom,

wherein at least one of (i), (ii) or (iii) comprises a backbone atom or a backbone pseudoatom;

(b) modifying one or more geometric constraints of said set of geometric constraints to produce a modified set of geometric constraints,

(c) comparing said modified set of geometric constraints to a data set of functional sites correlated with said biological function to determine whether said modified set of

geometric constraints compares positively with said data set of functional sites correlated with said biological function and, if there is a positive correlation; and

(d) repeating said modifying and comparing operations of steps b and c to modify one or more of said geometric constraints of said set of geometric constraints to an extent that said modified set of geometric constraints compares positively with said data set of functional sites correlated with said biological function without encompassing a predetermined amount of data sets not correlated with said biological function.

53. (Amended) A computer program product in a computer readable medium encoding a functional site descriptor, wherein the functional site descriptor defines at least one functional site of a protein, other than a divalent metal ion binding site, the functional site descriptor comprising:

(a) an amino acid residue identity constraint for a first amino acid residue of the functional site, wherein the first amino acid residue is identified as a single amino residue or as a subset of amino acid residues; and

(b) one or more geometric constraints between at least three different atoms, wherein each atom is in a different amino acid residue of the protein and the different atoms comprise:

(i) an atom of the first amino acid residue of the functional site, wherein the atom is selected from the group consisting of a backbone amide nitrogen, an alpha-carbon, a backbone carbonyl carbon, a backbone carbonyl oxygen, a backbone pseudoatom, and a beta-carbon;

(ii) an atom of a second amino acid residue of the functional site, wherein the atom is selected from the group consisting of a backbone amide nitrogen, an alpha-carbon, a backbone carbonyl carbon, a backbone carbonyl oxygen, a backbone pseudoatom, and a beta-carbon; and

(iii) an atom of a third amino acid residue of the protein, wherein the atom is selected from the group consisting of a backbone atom, a side chain atom, and a pseudoatom,

wherein at least one of (i), (ii) or (iii) comprises a backbone atom or a backbone pseudoatom.

54. (Amended) A computer implemented method for determining a functional site descriptor that defines a spatial configuration of a functional site, wherein the functional site descriptor defines a functional site of a protein other than a divalent metal ion binding site, the method comprising the following steps:

(a) identifying an amino acid residue identity constraint for a first amino acid residue of the functional site, wherein the first amino acid residue is identified as a single amino residue or as a subset of amino acid residues; and

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(b) identifying one or more geometric constraints between at least three different atoms, wherein each atom is in a different amino acid residue of the protein and the different atoms comprise:

(i) an atom of the first amino acid residue of the functional site, wherein the atom is selected from the group consisting of a backbone amide nitrogen, an alpha-carbon, a backbone carbonyl carbon, a backbone carbonyl oxygen, a backbone pseudoatom, and a beta-carbon;

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(ii) an atom of a second amino acid residue of the functional site, wherein the atom is selected from the group consisting of a backbone amide nitrogen, an alpha-carbon, a backbone carbonyl carbon, a backbone carbonyl oxygen, a backbone pseudoatom, and a beta-carbon; and

(iii) an atom of a third amino acid residue of the protein, wherein the atom is selected from the group consisting of a backbone atom, a side chain atom and a pseudoatom,

wherein at least one of (i), (ii) or (iii) comprises a backbone atom or a backbone pseudoatom, thereby determining a functional site descriptor.

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56. (Amended) A computer-implemented method for defining a functional site descriptor of a protein comprising the following steps:

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(a) identifying an amino acid residue identity constraint for a first amino acid residue of the functional site, wherein the first amino acid residue is identified as a single amino residue or as a subset of amino acid residues; and

(b) identifying one or more geometric constraints between at least three different atoms, wherein each atom is in a different amino acid residue of the protein and the different atoms comprise:

(i) an atom of the first amino acid residue of the functional site, wherein the atom is selected from the group consisting of a backbone amide nitrogen, an alpha-carbon, a backbone carbonyl carbon, a backbone carbonyl oxygen, a backbone pseudoatom, and a beta-carbon;

(ii) an atom of a second amino acid residue of the functional site, wherein the atom is selected from the group consisting of a backbone amide nitrogen, an alpha-carbon, a backbone carbonyl carbon, a backbone carbonyl oxygen, a backbone pseudoatom, and a beta-carbon; and

(iii) an atom of a third amino acid residue of the protein, wherein the atom is selected from the group consisting of a backbone atom, a side chain atom, and a pseudoatom,

wherein at least one of (i), (ii) or (iii) comprises a backbone atom, thereby defining the functional site descriptor.

57. (Amended) A computer program product in a computer readable medium for defining a functional site descriptor of a protein comprising a computer useable medium comprising a computer readable program code embodied therein, wherein the computer program product is capable of defining a functional site descriptor of a protein by a process comprising the following steps:

(a) identifying an amino acid residue identity constraint for a first amino acid residue of the functional site, wherein the first amino acid residue is identified as a single amino residue or as a subset of amino acid residues; and

(b) identifying one or more geometric constraints between at least three different atoms, wherein each atom is in a different amino acid residue of the protein and the different atoms comprise:

(i) an atom of the first amino acid residue of the functional site, wherein the atom is selected from the group consisting of a backbone amide nitrogen, an alpha-carbon, a

backbone carbonyl carbon, a backbone carbonyl oxygen, a backbone pseudoatom, and a beta-carbon;

(ii) an atom of a second amino acid residue of the functional site, wherein the atom is selected from the group consisting of a backbone amide nitrogen, an alpha-carbon, a backbone carbonyl carbon, a backbone carbonyl oxygen, a backbone pseudoatom, and a beta-carbon; and

(iii) an atom of a third amino acid residue of the protein, wherein the atom is selected from the group consisting of a backbone atom, a side chain atom, and a pseudoatom,

wherein at least one of (i), (ii) or (iii) comprises a backbone atom or a backbone pseudoatom, thereby defining the functional site descriptor.